

Numerical Detection of the Ergodicity Breaking in a Lattice Glass Model

Munetaka Sasaki*

Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan

Koji Hukushima

Department of Basic Science, The University of Tokyo, Tokyo 153-8902, Japan

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We directly detect the ergodicity breaking in a lattice glass model by a numerical simulation. The obtained results nicely agree with those by the cavity method that the model on a regular random graph exhibits a dynamical transition with the ergodicity breaking at an occupation density. The present method invented for a numerical detection of the ergodicity breaking is applicable to glassy systems in finite dimensions.

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Glass is a jammed state that particles can not move freely because they are densely packed. As the occupation density of particles increases, the system explores the phase space more and more slowly, and it eventually stop exploring the whole phase space. This impossibility for the system to explore the whole phase space is called ergodicity breaking. Although it is highly controversial whether real glasses in a finite dimension exhibit a dynamical glass transition with the ergodicity breaking or not, several theories of the glass predict the existence of the ergodicity breaking. The so-called random-first-order-transition theory [1–3] is one of them. This theory predicts that a single huge liquid state is broken up into exponentially large number of metastable amorphous solid states at a certain density (or temperature) so that the structural entropy or the complexity becomes finite. The (free-)energy barriers among the states become infinite in the thermodynamic limit and the ergodicity is broken there. Detailed analyses in statistical mechanics with the cavity method [4, 5] indicate that the Biroli-Mézard (BM) lattice glass model [6] defined on a regular random graph exhibits the ergodicity breaking [7, 8] in accordance with the random-first-order-transition scenario. A series of studies with the cavity method also indicate that many constraint-satisfaction problems exhibit an analogous clustering transition of solutions (see [5] and references therein). However, it is still an open problem whether there exists the ergodicity breaking in these systems because the cavity method is based on several non-trivial assumptions (see chapter 19 of Ref. [5]) and it does not directly observe the structure of the phase space. Therefore, it is desirable to verify the existence of the ergodicity breaking by a numerical simulation to check the validity of the previous studies. Furthermore, to study the ergodicity breaking in finite-dimensional systems, a proper numerical method is indispensable because analytical methods such as the cavity method are not available there.

In the present study, we investigate the BM lattice glass model on a regular random graph by Monte-Carlo

(MC) simulation with the aim of a direct detect of the ergodicity breaking. By properly designing the method and adopting a list-referring MC method [9] and the Wang-Landau method [10, 11] for an efficient exploration of the phase space, we succeeded in directly detecting the ergodicity breaking. Our results nicely agree with those by the cavity method that the model exhibits a dynamical transition with the ergodicity breaking at an occupation density $\rho_d = 0.5708$.

Model.— The BM model is a kind of lattice glass models. A binary variable σ_i is defined on each site. The variable σ_i denotes whether a site i is occupied by a particle ($\sigma_i = 1$) or not ($\sigma_i = 0$). In this study, we consider the BM model defined on a regular random graph. Each site is connected with k neighbouring sites which are chosen randomly from all of the sites. A particle configuration $\{\sigma_i\}$ is restricted by hard constraints that neighbouring occupied sites of each particle should be less than or equal to l . The BM model is characterized by the two integers k and l , which satisfy the inequality $k > l$. The probability distribution of the BM model for a particle configuration $\{\sigma_i\}$ is given as

$$P\{\sigma_i\} = Z^{-1} C\{\sigma_i\} W\{\sigma_i\}. \quad (1)$$

In this equation, Z is the partition function defined by $Z \equiv \text{Tr}_{\{\sigma_i\}} C\{\sigma_i\} W\{\sigma_i\}$ and $C\{\sigma_i\}$ is an indicator function which is one if $\{\sigma_i\}$ satisfies all of the constraint conditions or zero otherwise. $W\{\sigma_i\}$ is a weight of the particle configuration $\{\sigma_i\}$. For example, in the case of the grand-canonical ensemble, $W\{\sigma_i\}$ is given as $W\{\sigma_i\} = \exp[\mu N\{\sigma_i\}]$, where μ is a chemical potential, $N\{\sigma_i\} \equiv \sum_{i=1}^{N_{\text{site}}} \sigma_i$, and N_{site} is the number of sites.

In the present study, we will focus on the BM model on a regular random graph with $k = 3$ and $l = 1$. The phase space structure of the model indicated by detailed analyses based on the cavity method [7, 8] is briefly illustrated in Fig. 1. The model exhibits a dynamical transition at an occupation density $\rho_d = 0.5708$. The phase space is divided into numerous clusters at this density and the ergodicity is broken there. However, no static anomaly

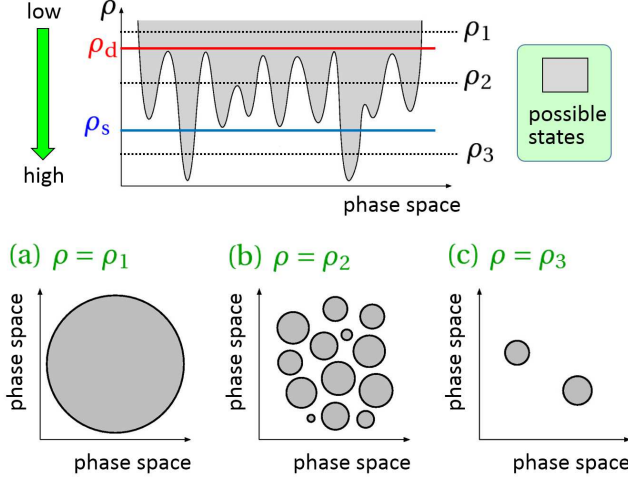


FIG. 1: (Color online) A schematic illustration of the phase space structure of the BM model indicated by the previous studies [7, 8]. The gray region denotes possible states (particle configurations) which satisfy all of the constraint conditions. The vertical and horizontal axes of the top figure are the occupation density ρ and the phase space, respectively. The three bottom figures are cross sections of the top figure at (a) $\rho = \rho_1$, (b) $\rho = \rho_2$, and (c) $\rho = \rho_3$, respectively, where $\rho_1 < \rho_d < \rho_2 < \rho_s < \rho_3$. One huge cluster is divided into numerous clusters at a dynamical transition density ρ_d , and the number of clusters becomes of order one at a static transition density ρ_s .

is detected at ρ_d . As the density further increases, the number of clusters decreases and it finally becomes of order one at an occupation density $\rho_s = 0.5725$. A static transition with a one-step replica symmetry breaking occurs at this density. The purpose of the present study is to directly detect the dynamical transition with the ergodicity breaking by a numerical simulation.

Basic strategy.— Figure 2 shows a schematic illustration of a simulation to detect the ergodicity breaking. In the present study, we perform a simulation in which the occupation density ρ is restricted to be $\rho_L \leq \rho \leq \rho_U$. Therefore, the system can only explore the gray region in the figures. The upper occupation density ρ_U is fixed to a certain value above the static transition density $\rho_s = 0.5725$ evaluated by the cavity method, while the lower occupation density ρ_L is changed across ρ_d .

To judge whether an ergodicity breaking is induced by the change in ρ_L or not, we measure the probability distribution of the overlap $P(q)$ between two states. We therefore perform simulations for two replicas. The two replicas have the same initial state and their particle configurations are updated independently with different random number sequences. The overlap q is calculated from two states at the upper occupation density ρ_U . In this measurement, we can expect that $P(q)$ exhibits the following ρ_L dependence: When (a) $\rho_L < \rho_d$, the system can

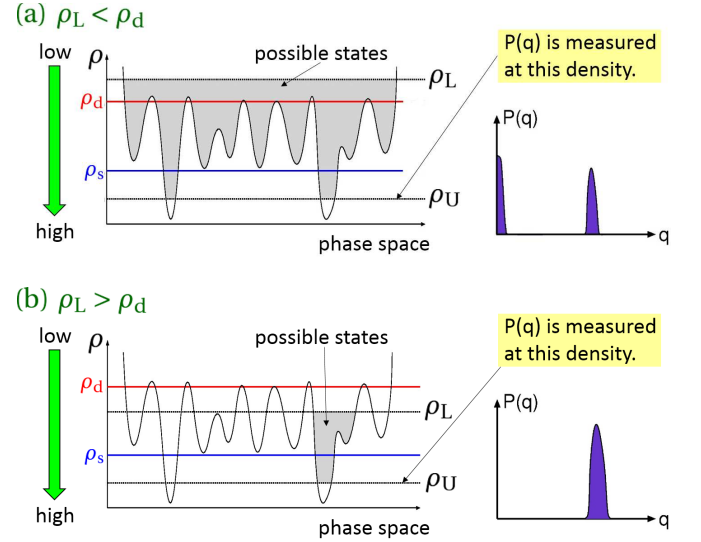


FIG. 2: (Color online) A schematic illustration of a simulation to detect the ergodicity breaking. The system can explore the gray regions in the left two panels under the restriction $\rho_L \leq \rho \leq \rho_U$. The simulation is performed for two replicas to measure the probability distribution of the overlap $P(q)$. The overlap q is measured at ρ_U . Two replicas have the same initial particle configuration. When (a) $\rho_L < \rho_d$, the system can explore the whole phase space when it reaches low density region. Therefore, the two replicas can be in either the same valley or different ones. In contrast, when (b) $\rho_L > \rho_d$, two replicas can never escape from the common initial valley. The right two panels show expected $P(q)$'s in the two cases.

explore the whole phase space when it reaches low density region (see the top left panel in Fig. 2). Therefore, two replicas can be in either the same valley or different ones. As a result, $P(q)$ has two peaks around 0 and 1 (see the top right panel). In contrast, when (b) $\rho_L > \rho_d$, $P(q)$ has a single peak around 1 because two replicas can never escape from the common initial valley.

Devices for an efficient exploration of the phase space.— Following the protocol mentioned above, there is a possibility to misjudge the occurrence of the ergodicity breaking because of insufficient exploration of the phase space in numerical simulations. To reduce the possibility, the phase space should be explored as efficiently as possible. We therefore devised the simulation method in the following two points: Firstly, we used an efficient list-referring MC (LRMC) method [9]. The basic idea of the LRMC method is similar to that of the N -fold way method [12]. By using a list of sites into which we can insert a particle, we avoid trying a useless transition which is forbidden by the constraint conditions. It is demonstrated in Ref. 9 that the relaxation time of the LRMC method is about 10^3 times shorter than that of the standard MC method in some cases. Secondly, we measured the density of states (DOS) and utilized it for an efficient

measurement of $P(q)$. To be specific, when we measure $P(q)$, we perform a MC simulation in which the weight $W\{\sigma_i\}$ in Eq. (1) is given as

$$W\{\sigma_i\} = \frac{1}{\Omega(N\{\sigma_i\})}, \quad (2)$$

where Ω is the DOS defined by

$$\Omega(N') \equiv \text{Tr}_{\{\sigma_i\}} \delta_{N', N\{\sigma_i\}} C\{\sigma_i\}. \quad (3)$$

We adopted this weight so that the probability $P(N')$ of the number of particles being N' , which is defined by

$$P(N') \equiv \text{Tr}_{\{\sigma_i\}} \delta_{N', N\{\sigma_i\}} P\{\sigma_i\}, \quad (4)$$

does not depend on N' . By visiting all of densities between ρ_L and ρ_U with an equal probability, the system can explore the phase space efficiently. The DOS $\Omega(N')$ is numerically calculated by the Wang-Landau method [10, 11], which is one of the standard methods for the DOS calculation. As demonstrated in Ref. 9, the performance of the Wang-Landau method is significantly improved with the combined use of the LRMC method.

Procedures of the simulation.— In the present simulation, we first perform a simulated annealing MC in the grand-canonical ensemble to find a particle configuration with the occupation density ρ_U . In this calculation, the chemical potential μ is gradually increased from 0 to 12.5 by 0.1, and a particle configuration with a maximum occupation density is recorded. Because the maximum occupation density obtained by simulations is larger than ρ_U in almost all cases, we can create a particle configuration with the density ρ_U by deleting a few particles at random. This particle configuration is used as an initial state in both the subsequent DOS calculation and the $P(q)$ measurement. We next calculate the DOS $\Omega(N')$ within $\rho_L \leq \rho \leq \rho_U$ by the Wang-Landau method. The DOS is calculated for each sample of a random graph.

After these two steps, we perform a simulation for the $P(q)$ measurement with the weight Eq. (2). To measure $P(q)$ at ρ_U , we update the particle configurations of the two replicas in a sequential manner: We first update the particle configuration of the first replica until the following two conditions are satisfied:

- The occupation density is ρ_U .
- The elapsed time from the previous measurement is larger than one MC step.

The second condition is imposed to avoid a successive measurement. We then update the particle configuration of the second replica until the two conditions are satisfied. After that, we calculate the overlap q from the particle configurations of the two replicas $\{\sigma_i^{(1)}\}$ and $\{\sigma_i^{(2)}\}$, where q is defined by

$$q \equiv \frac{1}{C_N} \sum_i (\sigma_i^{(1)} - \rho_U)(\sigma_i^{(2)} - \rho_U), \quad (5)$$

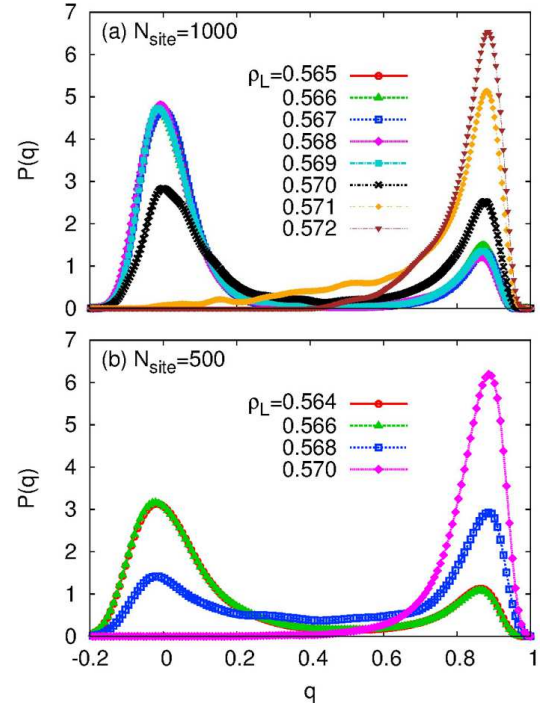


FIG. 3: (Color online) ρ_L dependence of $P(q)$ for (a) $N_{\text{site}} = 1000$ and (b) $N_{\text{site}} = 500$. The values of ρ_U for $N_{\text{site}} = 1000$ and $N_{\text{site}} = 500$ are 0.573 and 0.572, respectively. The average over random graphs is taken over 100 samples.

with $C_N \equiv N_{\text{site}}\rho_U(1 - \rho_U)$ being a normalization factor. The value of q is close to one if the two particle configurations are similar, and it is close to zero if there is no correlation between them. This sequential update of the two replicas and the subsequent calculation of q is repeated again and again to measure $P(q)$. The simulation is performed until the average of the MC steps of the two replicas becomes larger than 5×10^7 . The first 1.25×10^7 MC steps are for the equilibration. $P(q)$ is calculated in the subsequent 3.75×10^7 MC steps.

Dynamical rules.— Because the ergodicity is the possibility for a system to explore the phase space, it clearly depends on dynamical rules on which the system explores the phase space. As mentioned above, we update the particle configuration with the LRMC method. In this method, the particle configuration is changed one by one by either inserting or deleting a particle stochastically [13]. An insertion or deletion site is chosen randomly from all of the sites at which we can insert or delete a particle. In the present study, we investigate the ergodicity breaking on this dynamical rule restricted to the single-particle update.

Results.— Figure 3(a) shows the ρ_L dependence of $P(q)$ for $N_{\text{site}} = 1000$. The average over random graphs is taken over 100 samples. ρ_U is fixed to 0.573, which is slightly above the static transition density $\rho_s = 0.5725$ evaluated by the cavity method. In contrast, ρ_L is

changed from 0.565 to 0.572 by 0.001. Because N_{site} is 1000, this is the minimal increment of ρ_L . When $\rho_L \leq 0.569$, $P(q)$ hardly depends on ρ_L and all of the data collapse into each other. As expected, $P(q)$ has two peaks around 0 and 1 (see the top right panel in Fig. 2). However, the shape of $P(q)$ abruptly changes at $\rho_L = 0.570$. It is surprising that such a distinct change in $P(q)$ is induced by a minimal change in ρ_L . The peak around zero completely disappears when $\rho_L = 0.571$ and 0.572. We emphasize that these changes in $P(q)$ are caused solely by the ergodicity breaking because $P(q)$ is always measured at the fixed upper occupation density $\rho_U = 0.573$. These observations strongly support that the model exhibits the ergodicity breaking at around $\rho_d = 0.571$, consistent with the previous result by the cavity method.

We next turn to the result of $N_{\text{site}} = 500$ shown in Fig. 3(b). In the simulation, ρ_L is changed from 0.564 to 0.570 by 0.002, which is the minimal increment for $N_{\text{site}} = 500$. ρ_U is fixed to 0.572. We see that $P(q)$ shows a qualitatively similar ρ_L dependence to that for $N_{\text{site}} = 1000$. However, there are several quantitative difference between them: Firstly, an abrupt change in $P(q)$ occurs at a lower density $\rho_L = 0.568$. Secondly, $P(q)$ has a peak around one even in the ergodic case ($\rho_L \leq 0.566$) despite that ρ_U is slightly lower than ρ_s . We attribute these qualitative differences to a finite-size effect. In fact, we have found that the average of maximum densities measured in simulations *decreases* with decreasing N_{site} [9].

Figure 4 shows how the overlap q changes with MC time in the measurement of $P(q)$. In the figure, the overlap q measured in one sample is plotted as a function of the sum of the elapsed times of the two replicas. The number of sites N_{site} is 1000. The values of ρ_L are (a) 0.565 and (b) 0.572, respectively. A common sample is used for the two cases. When (a) $\rho_L = 0.565 < \rho_d$, q quickly drops to zero at the beginning and it repeats intermittent increases from zero to one. Therefore, $P(q)$ has two peaks in this ergodic case. On the contrary, q never drops to zero when (b) $\rho_L = 0.572 > \rho_d$.

Discussion and conclusions.— In the present study, we have examined the ergodicity breaking of the BM lattice glass model on a regular random graph, and obtained results which nicely agree with those of the cavity method. However, we consider that this agreement is not trivial from the following two points of view: (i) As mentioned above, the cavity method is based on several non-trivial assumptions. (ii) The details of the ergodicity breaking such as the transition density should in principle depend on dynamical rules, while they are not specified in the cavity method. It is an intriguing issue in the future to unveil how this agreement between our numerical results and the analyses based on the cavity method comes from. To this end, it may be helpful to investigate how the details of the ergodicity breaking depend on dynamical rules by using the present method.

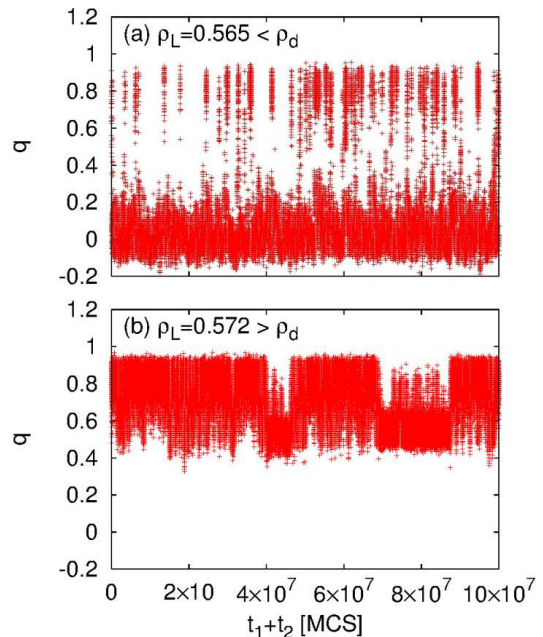


FIG. 4: (Color online) The overlap q measured at $\rho_U = 0.573$ in one sample is plotted as a function of the sum of the elapsed times of the two replicas. The number of sites N_{site} is 1000. The values of ρ_L are (a) 0.565 and (b) 0.572, respectively. A common sample is used for the two cases.

In conclusion, we have numerically investigated the ergodicity breaking in the BM lattice glass model on a regular random graph. As a result, we have obtained a strong evidence that an ergodicity breaking occurs around the dynamical transition density $\rho_d = 0.5708$ predicted by the cavity method. We can easily apply the present numerical method to lattice glass models in finite dimensions. We hope that the present study will stimulate further research on the ergodicity breaking in glassy systems.

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* Electronic address: msasaki@camp.apph.tohoku.ac.jp

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